

Fig. 1: Conceptual framework of the stochastic simulation approach, modified from [1].

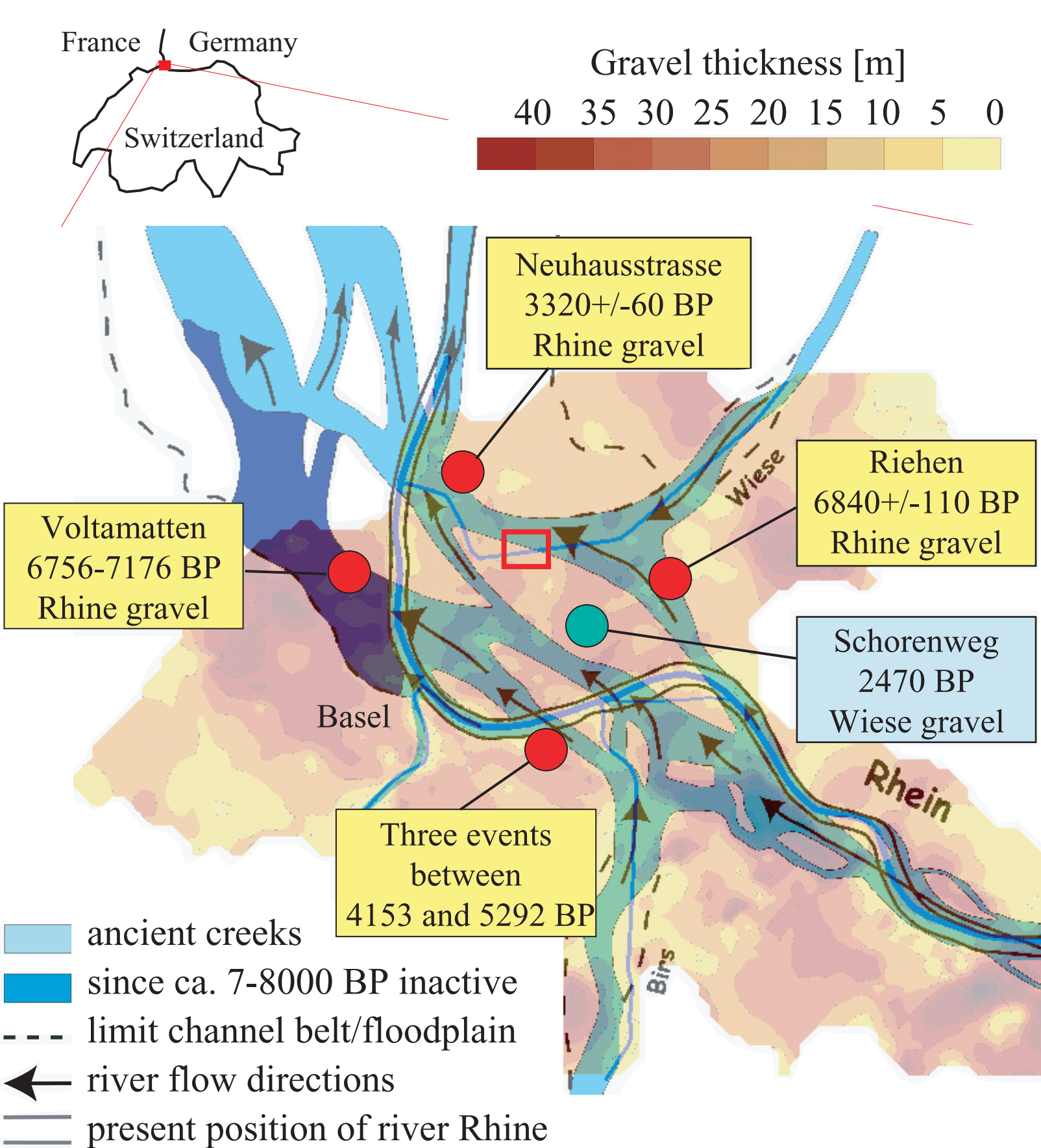


Fig. 2: Landscape development of the Basel area prior to human activity; study site bounded by the red.

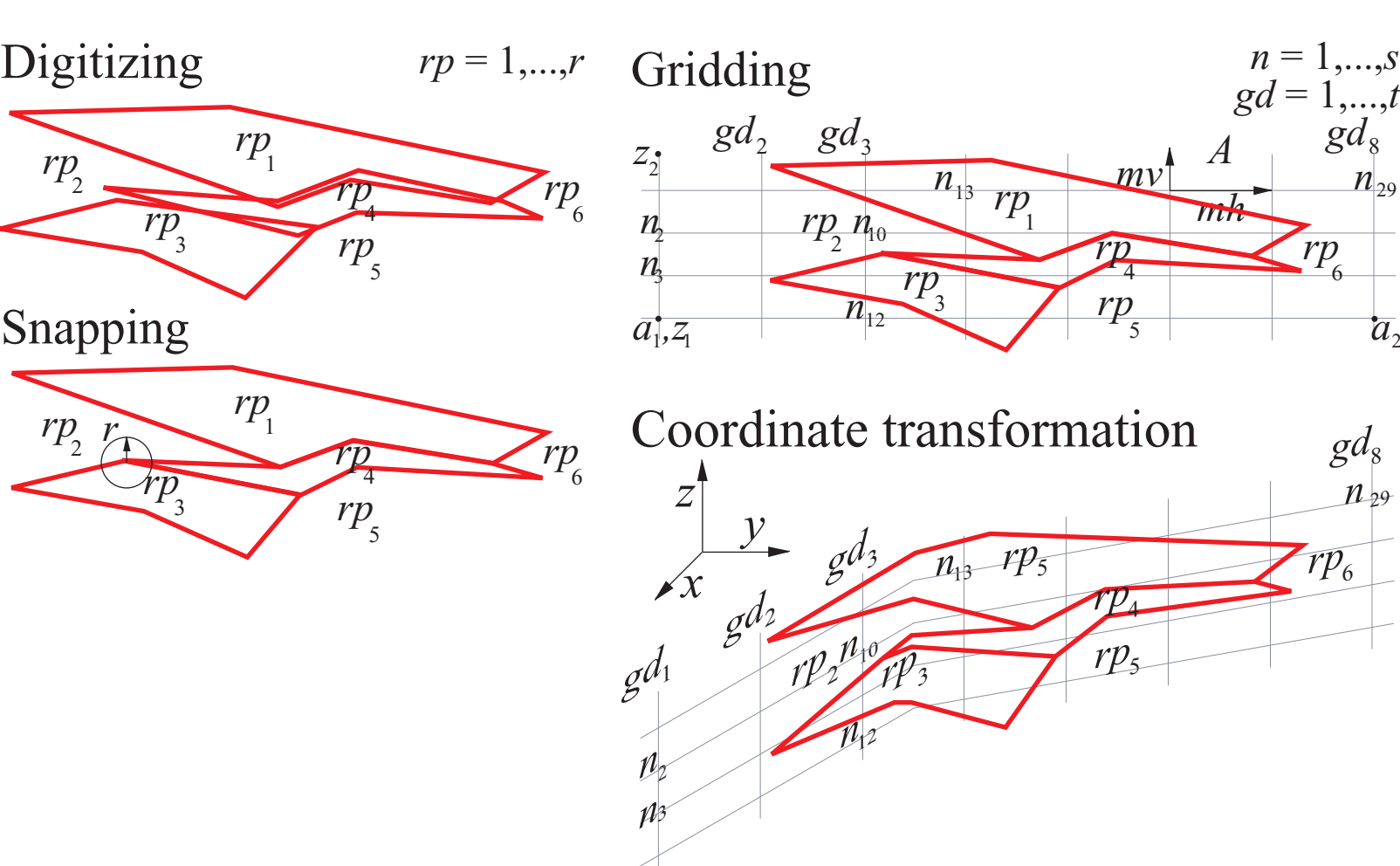
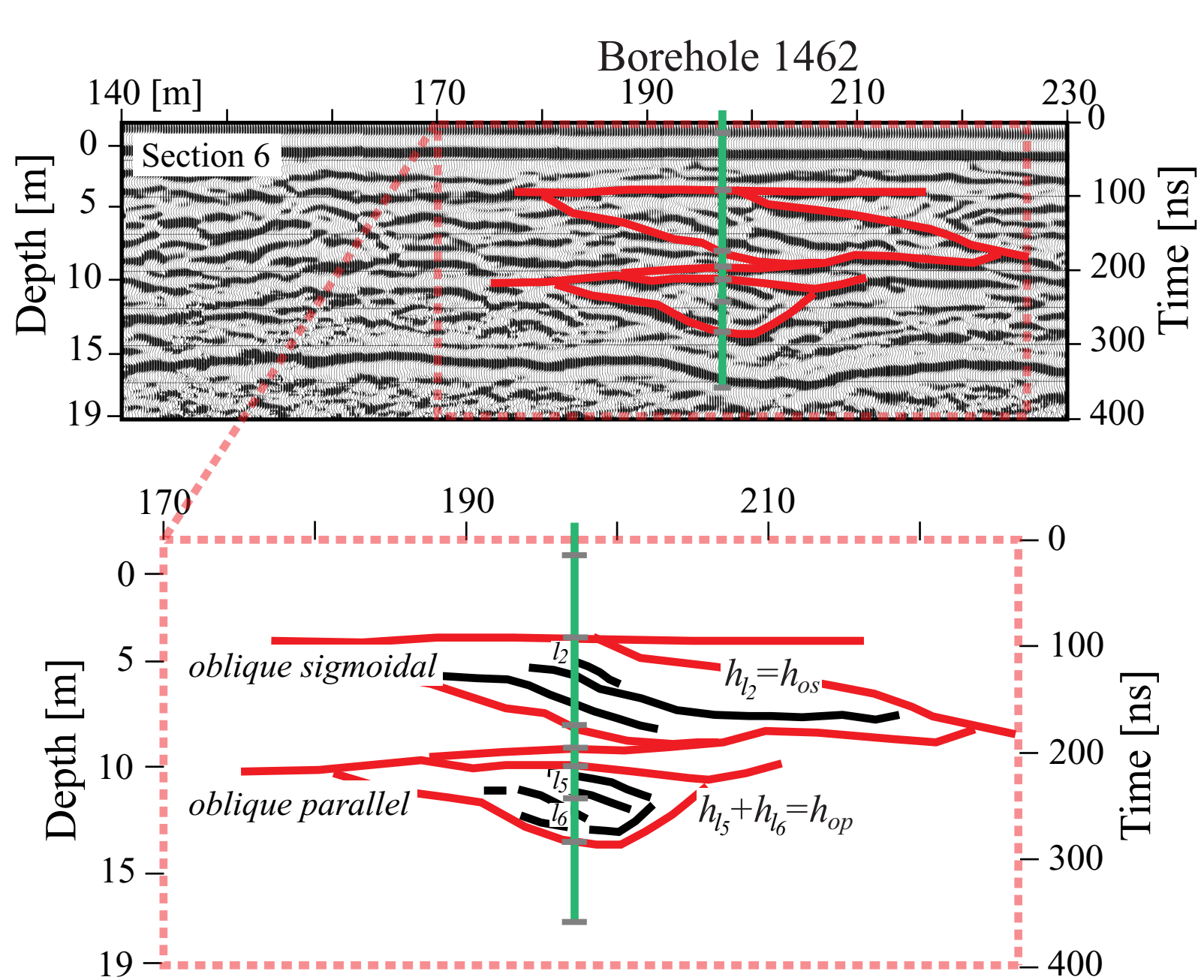


Fig. 3: Radarfacies analysis and processing of reflection pattern into point data.

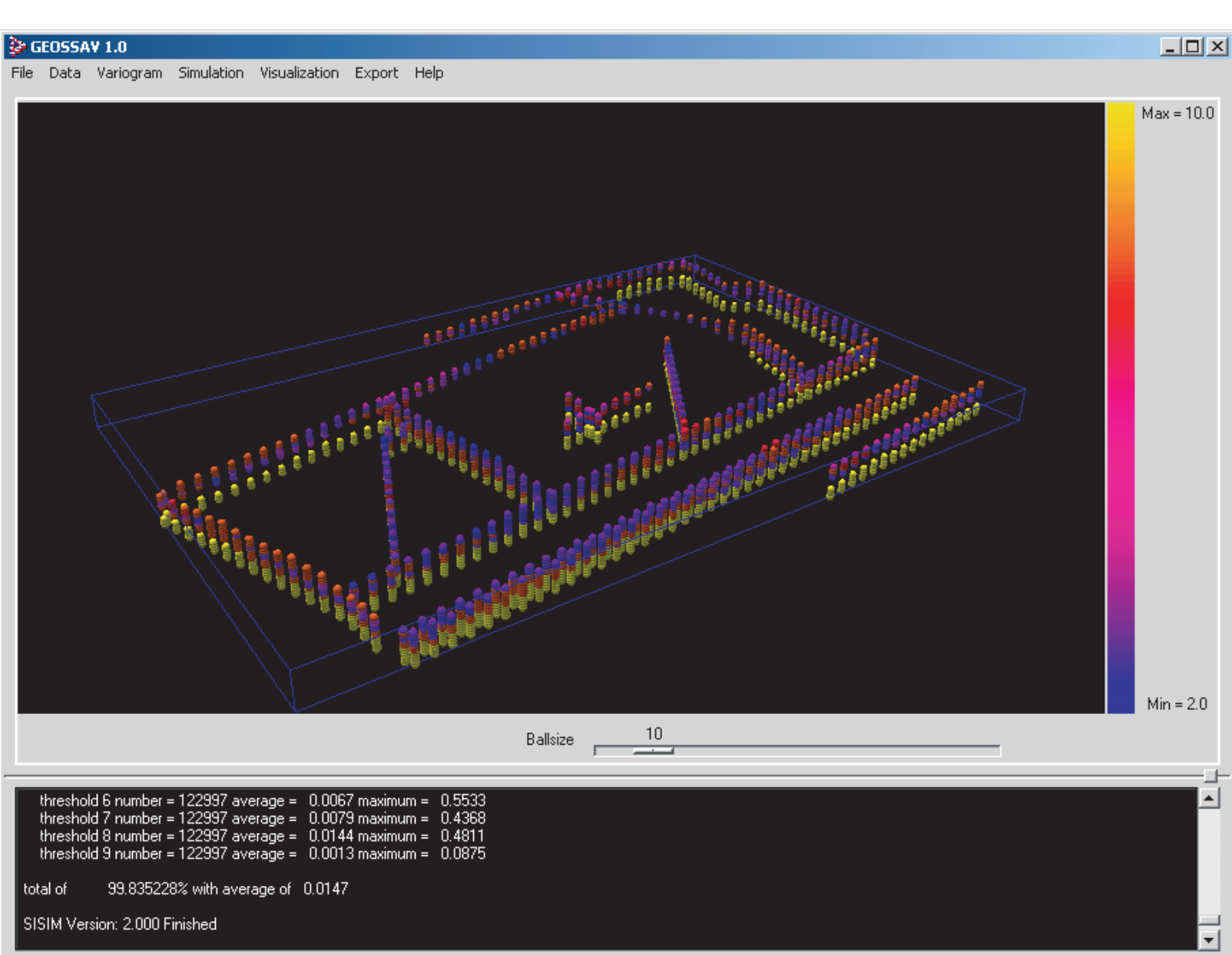


Fig. 4: Main GEOSSAV window with menu bar for pull-down menus, window for visualization, and window for error checking; study site bounded by the blue lines.

Introduction

For many practical hydrogeological problems such as determination of well capture zones or risk assessment of groundwater pollutants due to contaminated sites, not only statistical distribution of lithofacies is required but also site-specific structural information. The available information on heterogeneity, however, is mostly limited and typically of different quality (e.g., outcrop and core analyses, geophysical data). In addition, the quantitative integration of such diverse data types represents one of the major challenges in the field of subsurface characterization. To bridge this inherent gap in terms of resolution and coverage that exists between nature and probabilistic models (Fig. 1), we developed the software package GEOSSAV (Geostatistical Environment fOr Subsurface Simulation And Visualization) that combines geostatistical analysis, simulation, visualization, and data export for groundwater simulation systems [2]. In this paper, we begin by analyzing a part of the Rhine/Wiese aquifer near Basel, Switzerland. The resulting geological/geophysical database is then used as conditioning information for the realization of geostatistically controlled conductivity and porosity models that are used for the simulation of changes in the groundwater flow regime depending on hydrologic variations, water supply operation data, progress of river restoration, and subsurface heterogeneity. Finally, the integration platform and software resources of GEOSSAV are listed.

Geological/geophysical database

The study site is located in the ancient confluence of the main river Rhine and its tributary Wiese (Fig. 2). Detailed drill-core descriptions of five boreholes and georadar data from 14 vertical georadar sections (total length of all sections 3'040 m) have been examined in a range of 550 m x 400 m x 21 m (Figs. 2/3). The unconfined aquifer consists of Quaternary unconsolidated coarse alluvial deposits. Tertiary marls underlie these gravels. The aquifer thickness varies between 13 and 18 meters. The lower 80% of the aquifer consists of Rhine gravel and the upper 20% of Wiese gravel. Within these two stratigraphic units a number of sedimentary structures are recognized that were generated by sedimentary processes in the braided fluvial system [3, 4]. Lithofacies types associated with the sedimentary structures for this area include [5]: open-framework gravel (OW), open-framework/bimodal gravel couplets (OW/BM), gray gravel (GG), brown gravel (BG), alternating gray and brown gravel layers (GG/BG), horizontally layered or inclined, silty gravel (SG), sand lenses (SA), and silt lenses (SI). The lithofacies-based interpretation of the drill-core and georadar data [6] considers differences in data uncertainty and provides lithofacies type probabilities for points along boreholes and grid nodes with arbitrary mesh sizes in horizontal and vertical direction along georadar sections (Figs. 3/4).

Spatial statistics

For the variogram analysis the indicator transform at grid node location is set to 1 for the lithofacies types with the greatest probability values, 0 otherwise. Variogram information for the nine sedimentary structure types in the study area is given in Fig. 5. The main outcome of the variogram analysis is the orientation of the sedimentary structure types representing the main flow direction of the river Rhine in the lower part of the aquifer and the tributary Wiese in the upper part of the aquifer.

Aquifer characterization using sequential indicator simulation

The aquifer is simulated by sequential indicator simulation (Fig. 6). In Fig. 7 one realization of the sequential indicator simulation is shown with separate realizations for the lower and the upper parts of the aquifer. The regular model grid is defined by 110 x 80 x 10 cells for the lower part and by 110 x 80 x 1 cells for the upper part, respectively. Cell sizes are 5 m x 5 m x 1.5 m for the lower part, and 5 m x 5 m x 6 m for the upper part, respectively. The saturated thickness of the topmost layer, however, is about only 1-2 m. A total of ten combinations of sedimentary structure-type distributions were simulated. The resulting probability density functions of the sedimentary structure types deviate less than $\pm 10\%$ from the initial probability density functions. The generated sedimentary structures are characterized by randomly selecting hydraulic conductivity and porosity values (Fig. 8) given by means and variances in [7].

Groundwater modeling

For each aquifer realization, a flow model computation was performed and the capture zone for drinking water well 13 was approximately defined by particle tracking. By superposition of all produced capture zones a probability distribution is obtained that describes the probability of a point on the ground surface belonging to the capture zone. This probability is given by the fraction of capture zones among all realizations containing the point.

Fig. 9 shows probability distributions of the capture zone of drinking water well 13 for conditions before and after river restoration as well as for low river discharge, moderate and high floods. Fig. 9a represents the calibrated groundwater

Sedimentary structure type	OW	OW/BM	GG	BG	GG/BG	GG/BG	SG	SA	SI
Variogram parameter					horizontal	inclined			
Probability density function	0.02	0.05	0.16	0.05	0.50	0.05	0.02	0.14	0.01
Sill	0.13	0.12	0.18	0.115	0.13	0.13	0.045	0.18	0.13
Max. azimuth [°]	240	240	240	240	240	240	270	200	240
Max. horiz. range [m]	3	24	60	34	50	7	14	50	3
Min. horiz. range [m]	1.5	18	24	24	18	3	18	16	1.5
Vertical range [m]	0.5	4	6	5	6	1	4	3	0.5
Probability density function	0.02	0.06	0.12	0.05	0.50	0.05	0.03	0.16	0.01
Sill	0.1	0.095	0.155	0.055	0.1	0.1	0.04	0.17	0.1
Max. azimuth [°]	310	320	315	300	310	310	300	300	310
Max. horiz. range [m]	5	54	60	40	70	8	30	60	5
Min. horiz. range [m]	2	22	19	22	30	4	17	22	2
Vertical range [m]	1	10	5	11	10	2	10	8	1

Fig. 5: Variogram information of Rhine and Wiese gravel used for the sequential indicator simulation to define the geometric anisotropy of the sedimentary structure types.

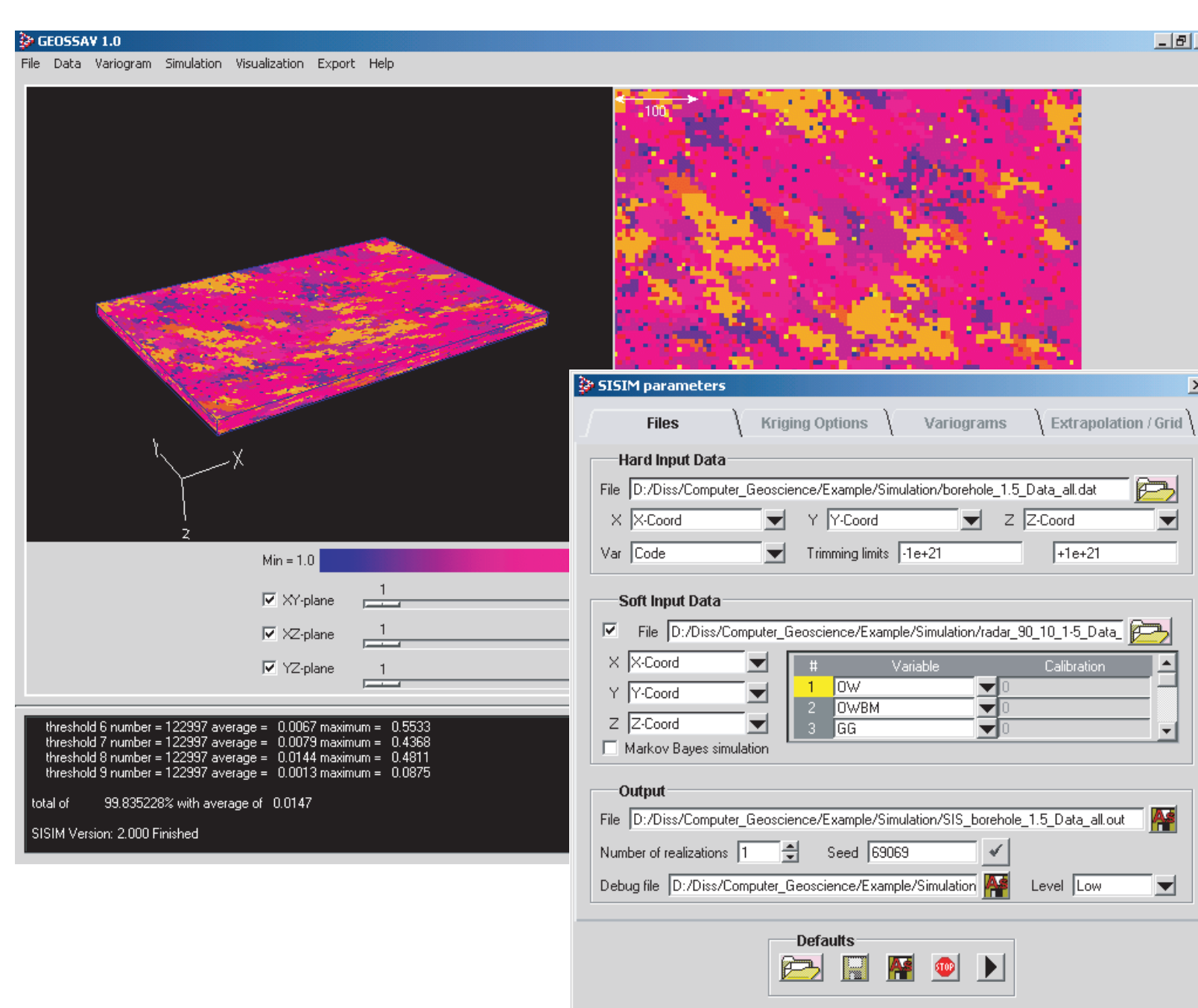


Fig. 6: Realization of sequential indicator simulation, visualized within OpenGL window, and a sectional detail of XY-plane; and dialog box for the sequential indicator simulation.

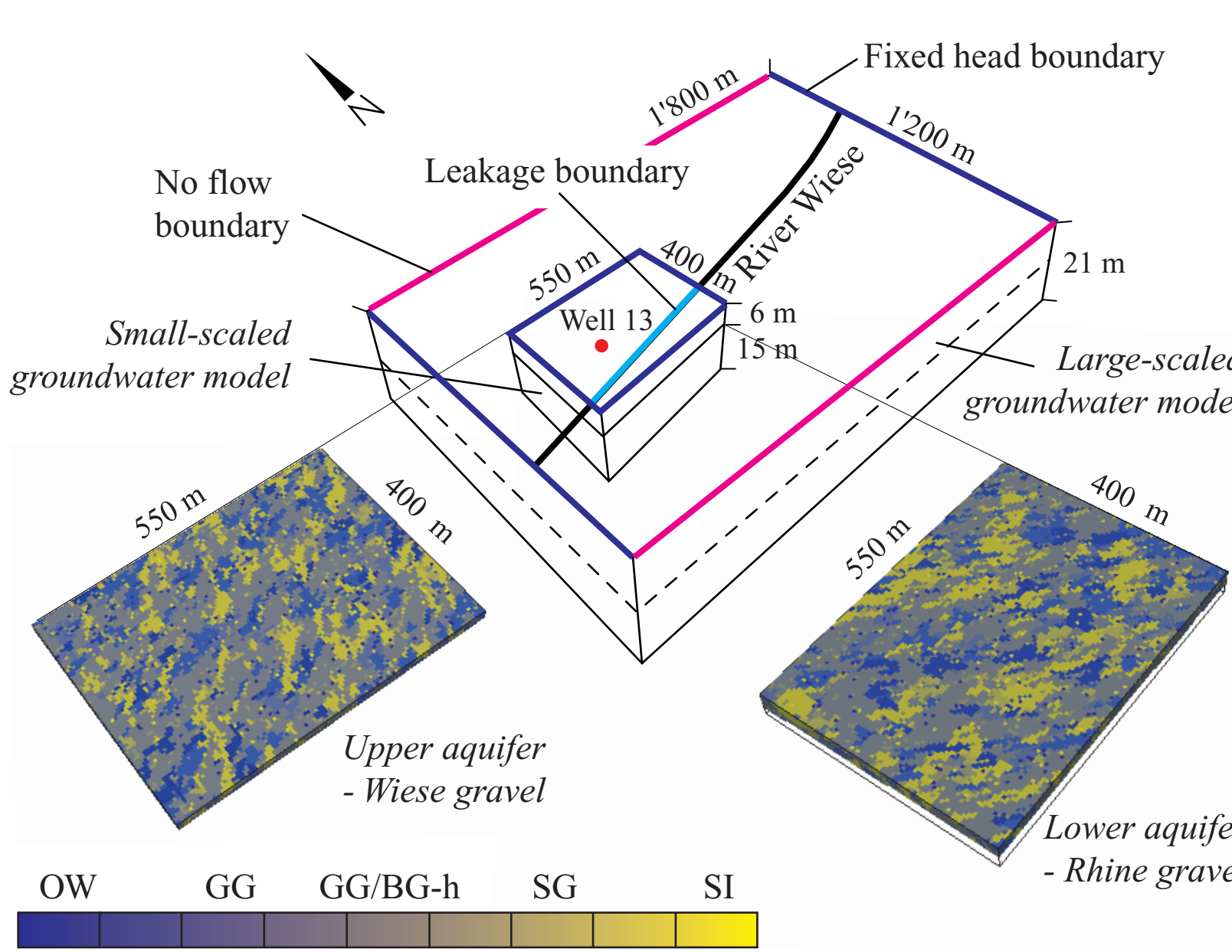


Fig. 7: Situation of small-scaled groundwater model, which relies on stochastically generated aquifer properties.

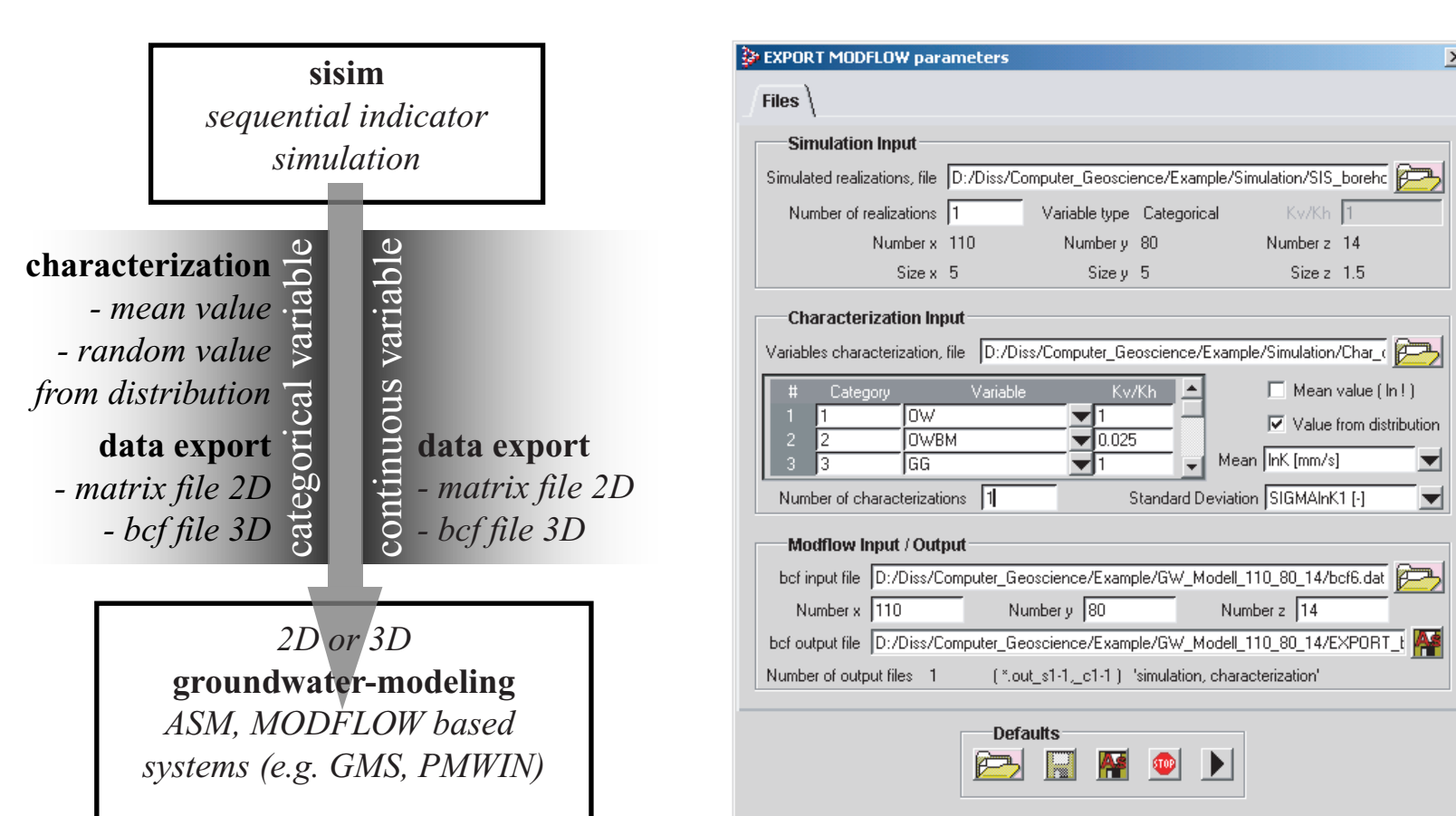


Fig. 8: Options for generating export files depending on the variable type used in the stochastic simulation, and dialog box for the export of block-centered flow (bcf) package files.

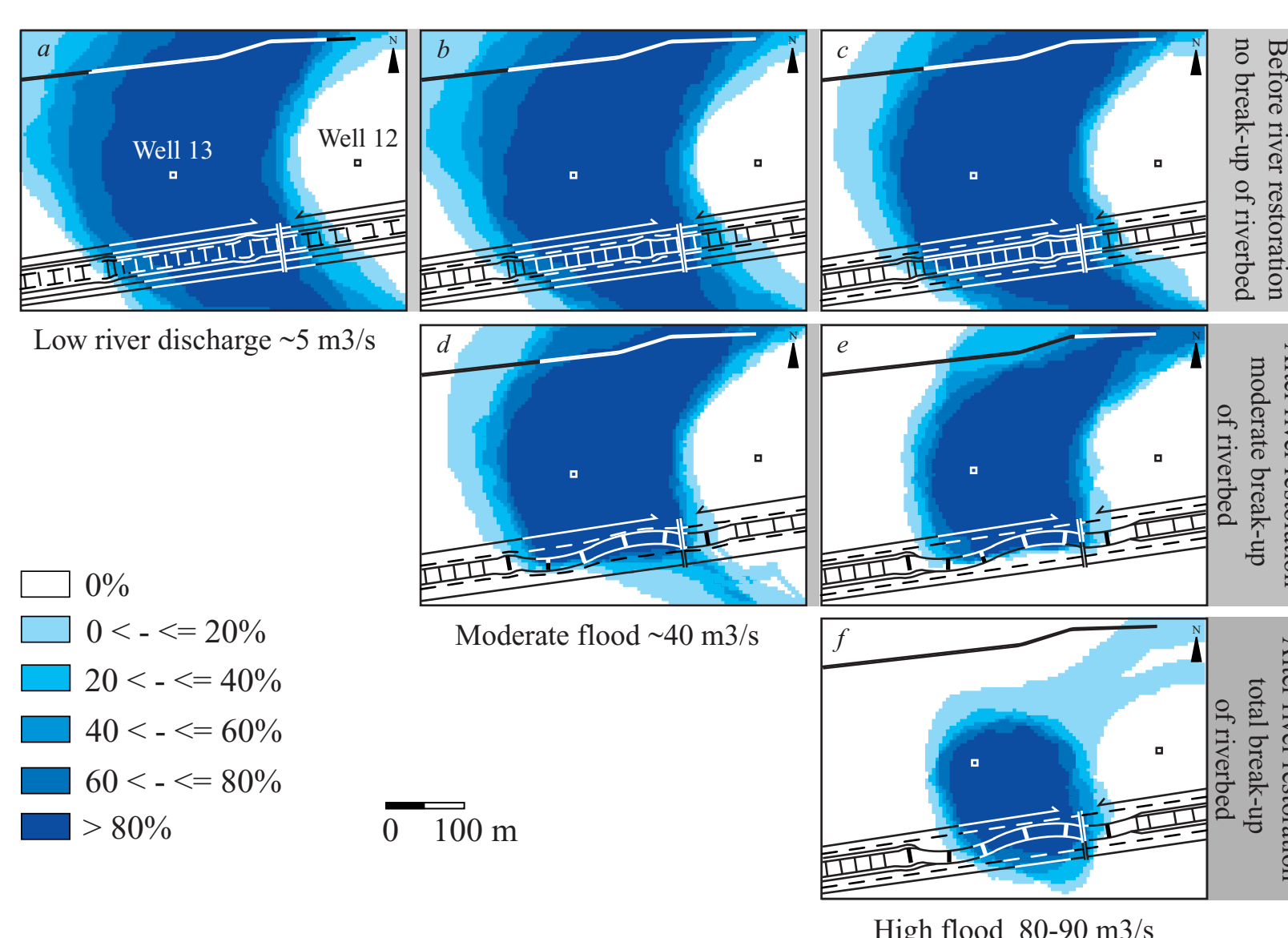


Fig. 9: Changes of the capture zone distribution of drinking water well 13 in the small-scaled groundwater model depending on river discharge, river restoration, water supply operation data, and subsurface heterogeneity.

model. The average of the mean squared deviations of observed versus calculated heads over the 10 flow simulations is 0.10 m². In Fig. 9b-f, predictions under changed boundary conditions are given, with each probability distribution representing the result of 10 flow and advective transport simulations. River restoration is simulated by increasing the leakage factor by a factor of 10 and 100, respectively, within the restored river channel, assuming moderate and strong increase of the hydraulic conductivity of the riverbed.

Integration platform and software resources of GEOSSAV

- GEOSSAV acts as an interface to selected geostatistical programs from the GSLIB [8], and can be used for data analysis (bicalib), variogram computation of regularly or irregularly spaced data (gamv, vargplt), and sequential indicator simulation of subsurface heterogeneities (sisim). Sequential indicator simulation, based on various kriging techniques (simple, ordinary, and Bayesian), is suitable for the simulation of either continuous variables such as hydraulic conductivity of an aquifer or chemical concentrations at a contaminated site, or categorical variables which indicate the presence or absence of a particular lithofacies.
- The data integration platform and development environment for GEOSSAV is Tcl/Tk. The standard OpenGL interface is used for rendering 3D data distributions and for slicing perpendicular to the main coordinate axis.
- Export options for finite-difference groundwater models allow either files that characterize single model layers or files that characterize the complete 3D flow model set-up for MODFLOW-based groundwater simulation systems [9, 10].
- GEOSSAV has been successfully tested on Microsoft Windows NT 4.0/2000/XP and on SuSE Linux 7.3. The current version is available at <http://www.unibas.ch/earth/pract>.

Conclusions

- GEOSSAV is a tool for the integration of hard and soft geological and geophysical data in the stochastic simulation and visualization of hydrogeological properties of the subsurface. The implemented software packages support subsurface characterization from data processing through simulation and visualization to model verification and data export to external finite-difference groundwater simulation systems. In particular GEOSSAV allows to model categorical and continuous variables such as lithofacies types and distributions of hydraulic properties. The distinguished lithofacies can be explained based on depositional processes (e.g. fluvial sediment sorting processes).
- The probability distribution of the well capture zone is strongly influenced not only by changing river discharge and riverbed structure, but also by subsurface heterogeneity. Preferential flow paths can be detected to some extent. In particular, zones along the riverbank with increased infiltration rates of river water can be recognized.
- Although the given example includes a characterization of the simulated geological structures by hydraulic parameters, GEOSSAV can definitely be used for other applications such as groundwater and/or soil contamination, site remediation, and ecology. In fact, whenever stochastic solutions are preferred to solve site-specific heterogeneity problems, GEOSSAV can be used as a user-friendly and adequate software solution.
- Due to the Tcl/Tk integration platform and development environment as well as the modular set-up, GEOSSAV can be easily upgraded and adapted to specific problems, which may be solved using geostatistical methods.

References

- Pannatier, Y., 1996. Variowin - Software for Spatial Data Analysis in 2D. Springer, New York.
- Regli, Ch., Rosenthaler, L., Huggenberger, P., 2004. GEOSSAV: a simulation tool for sub-surface applications. Computers & Geosciences 30, 221-238.
- Huggenberger, P., 1993. Radar facies: recognition of facies patterns and heterogeneities within Pleistocene Rhine gravels, NE Switzerland. In: Best, C.L., Bristow, C.S. (Eds.), Braided Rivers. Geological Society, Special Publication 75, 163-176.
- Siegenthaler, C., Huggenberger, P., 1993. Pleistocene Rhine gravel: deposits of a braided river system with dominant pool preservation. Best, C.L., Bristow, C.S. (Eds.), Braided Rivers. Geological Society Special Publication 75, 147-162.
- Regli, Ch., Rauber, M., Huggenberger, P., 2003. Analysis of aquifer heterogeneity within a well capture zone, comparison of model data with field experiments: A case study from the river Wiese, Switzerland. Aquatic Sciences 65, 111-128.
- Regli, Ch., Huggenberger, P., Rauber, M., 2002. Interpretation of drill-core and georadar data of coarse gravel deposits. Journal of Hydrology 255, 234-252.
- Rauber, M., Stauffer, F., Huggenberger, P., Dracos, T., 1998. A numerical three-dimensional conditioned/unconditioned stochastic facies type model applied to a remediation well system. Water Resources Research 34 (9), 2225-2233.
- Deutsch, C.V., Journel, A.G., 1998. GSLIB: Geostatistical Software Library and User's Guide. Oxford University Press, Oxford.
- Chiang, W.-H., Kinzelbach, W., 2001. 3D-Groundwater Modeling with PMWIN - A Simulation System for Modeling Groundwater Flow and Pollution. Springer, Berlin.
- Environmental Modeling Systems Inc., 2002. GMS: Groundwater Modeling System. <http://www.ems-i.com>.

Acknowledgments

This work was financially supported by the Swiss National Science Foundation and the University of Basel.